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UNITARITY IN ONE DIMENSIONAL NONLINEAR QUANTUM CELLULAR AUTOMATA

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ABSTRACT

Unitarity of the global evolution is an extremely stringent condition on finite state models in discrete spacetime. Quantum cellular automata, in particular, are tightly constrained. In previous work we proved a simple No-go Theorem which precludes nontrivial homogeneous evolution for linear quantum cellular automata. Here we carefully define general quantum cellular automata in order to investigate the possibility that there be nontrivial homogeneous unitary evolution when the local rule is nonlinear. Since the unitary global transition amplitudes are constructed from the product of local transition amplitudes, infinite lattices require different treatment than periodic ones. We prove Unitarity Theorems for both cases, expressing the equivalence in $1+1$ dimensions of global unitarity and certain sets of constraints on the local rule, and then show that these constraints can be solved to give a variety of multiparameter families of nonlinear quantum cellular automata. The Unitarity Theorems, together with a Surjectivity Theorem for the infinite case, also imply that unitarity is decidable for one dimensional cellular automata.

KEY WORDS: Quantum cellular automaton; nonlinear dynamics; unitarity.

1. Introduction

Already present in Feynman's inspirational essay on quantum physics and computation [1] is the concept of a binary quantum cellular automaton (QCA): a discrete spacetime array of quantum processors, each of which has two eigenstates (un/occupied or spin up/down) and is coupled to some set of neighboring processors. He explicitly recognizes the difficulties of reconciling discreteness and locality of interaction with Lorentz invariance—the same problem which must be solved in the causal set approach to quantum gravity [2]. Grössing, Zeilinger, *et al.*, discovered a similar conflict with group invariance in their attempts to apply QCAs as quantum simulators, *i.e.*, for quantum rather than deterministic computation.* Being unable to reconcile discreteness and locality with translation invariance and unitarity, they were led to study a class of CAs whose evolution is, although 'probability' preserving, both nonunitary [6] and nonlocal [7].

Near the beginning of our investigation into exactly unitary—and therefore truly quantum—CAs we proved that these physically reasonable requirements are actually incompatible for this class of CAs. More precisely, taking the definition of QCA to include unitarity, discreteness and locality, we proved [8]:

No-go Theorem. *No nontrivial homogeneous linear binary QCA exists on Euclidean lattices in any dimension.*

We showed, however, that weakening the homogeneity condition slightly to require invariance under only a subgroup of translations allows the existence of linear binary QCAs [9]. The simplest of these *partitioned* [10] QCAs models the evolution of a quantum particle and, in the appropriate limit, simulates the $1+1$ dimensional Dirac equation. This physical interpretation motivates two reformulations of the QCA [9]:

> As a quantum lattice gas automaton. The QCA may be formulated as a lattice gas with a single particle. Generalizing to multiple particles forces the automaton to be nonlinear if we impose an exclusion principle. The dimension of the Hilbert (Fock) space of the theory is now exponential in the cardinality of the lattice. If there is no particle creation/annihilation, the one particle sector of the Fock space is equivalent to the original QCA.
>
> As a homogeneous linear ternary QCA. In the Dirac equation the amplitudes for the particle to be left/right moving at a point are combined into a two component field. Equivalently, the QCA may be formulated to have three eigenstates at each cell, corresponding to empty, left moving, and right moving. Coupling two copies of the original QCA makes the new one homogeneous.

Both generalizations evade the No-go Theorem; the first by being both nonlinear and not quite homogeneous and the second by being ternary.

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* Feynman [3], Margulis [4], and more recently, Lent and Tougaw [5] have investigated the possiblilities for deterministic computation using QCAs.

Emulating Morita and Harao's construction of a computation universal reversible one dimensional CA [11], Watrous has recently constructed a one dimensional QCA which is quantum computation universal [12] in the sense that it efficiently simulates the universal quantum Turing machine defined by Bernstein and Vazirani [13], which in turn efficiently simulates any quantum Turing machine as originally defined by Deutsch [14]. Both Morita and Harao's and Watrous' universal CAs are homogeneous, but since each may be considered to consist of three coupled partitioned CAs,* they may also be described as partitioned. They are not, therefore, binary—far more eigenstates are required. Since a primary motivation for considering QCA models for quantum computation is the likelihood that massive parallelism will optimize nanoscale computer architecture [16] and the most plausible nanoscale devices have only a few eigenstates [17], it is of interest to ask if the No-go Theorem may also be evaded by homogeneous *nonlinear* binary QCAs. In this paper we answer that question affirmatively and, as a first step toward exploring the computational power of such architectures, we explicitly parameterize the rule spaces for the simplest such QCAs.

We begin in Section 2 by carefully defining what it means for a CA to be quantum mechanical. Rather than restricting a QCA to have only finite configurations as do Watrous [12] and Dürr, Thanh and Santha [18], we consider both periodic and infinite lattices. In order for the global transition amplitudes to be well defined as the product of local transition amplitudes we must distinguish more carefully between these two situations than is necessary in the deterministic case. The distinction is emphasized in the following section by the observation that infinite QCAs must be asymptotically deterministic, though not necessarily quiescent.

In Section 3 we prove a series of results expressing the equivalence of unitary global evolution and sets of constraints on the local transition amplitudes. Utilizing a bijection between configurations/pairs of configurations and paths on weighted graphs G_1/G_2 we prove Unitarity Theorems 3.9 and 3.10. These show that unitarity is equivalent to sets of constraints on the weights of such paths arising from the condition that the global evolution be norm preserving and, in the infinite case, from the additional independent condition that the global evolution be surjective; the latter is the content of Surjectivity Theorem 3.18.

We observe in Section 4 that the Unitarity and Surjectivity Theorems, together with the finiteness of the graphs G_1 and G_2, prove that unitarity is decidable in one dimension. Dürr and Santha have obtained the same result by different methods [19]. Our main interest in this section, however, is to extract from these theorems a procedure for finding multiparameter families of local rules which define QCAs. We do so, and apply it in the cases where the local neighborhood has size 2 or 3.

At the beginning of Section 5 we show that a pattern observed in the derivation of

* Morita subsequently constructed a simpler universal reversible one dimensional CA which comprises two coupled partitioned CAs [15]; presumably the analogous construction also works in the quantum context.

the small local neighborhood rules in Section 4 generalizes to give families of QCAs for any size local neighborhoods. We conclude by discussing connections with deterministic reversible CAs and point in directions for further research to explore the computational power and physical interpretation of nonlinear QCAs.

2. Definitions

A homogeneous CA is defined by a 4-tuple (L, Q, f, E): For the purposes of this paper we will take the *lattice of cells* L to be the integers $\mathbb{Z}$ (possibly with periodic identifications to $\mathbb{Z}_N$); such a CA is *one dimensional*. Q is a finite set of *states* $\{0,\ldots,q-1\}$; *configurations* are maps $\sigma : L \to Q$, the argument of which will be denoted by a subscript. The *local rule* $f : Q \times Q^k \to \mathbb{C}$ defines the dynamics of the CA which it will be convenient to encode as a set of *amplitude vectors*: for each *local configuration* $\lambda = (i_1,\ldots,i_k) \in Q^k$,

$$|\lambda\rangle\!\rangle := \big(f(0|i_1,\ldots,i_k),\ldots,f(q-1|i_1,\ldots,i_k)\big) \in \mathbb{C}^q.$$

We use the variation $|\cdot\rangle\!\rangle$ of the familiar Dirac notation [20] to denote a vector in $\mathbb{C}^q$ while distinguishing it from a state vector of some quantum system. The sesquilinear inner product on $\mathbb{C}^q$ is denoted $\langle\!\langle\cdot|\cdot\rangle\!\rangle$. Also, the notation for the arguments of f has been chosen to evoke that of conditional probability so that $f(i|\lambda)$ is the i^{th} component in the amplitude vector, given that λ is the local configuration.

If the range of f is $\{0, 1\} \subset \mathbb{C}$ and each amplitude vector has exactly one nonzero component, the CA is *deterministic*: there is a *global evolution map* $F : L^Q \to L^Q$ defined by

$$\sigma' = F\sigma \quad\iff\quad \forall x \in L,\ f(\sigma'_x|\sigma_{x+E}) = 1, \tag{2.1}$$

where the *local neighborhood* $E := \{e_1,\ldots,e_k\}$ is a finite set of lattice vectors which defines the *E-subconfigurations* $\sigma_{x+E} := (\sigma_{x+e_1},\ldots,\sigma_{x+e_k}) \in Q^k$. F is well defined since for each E-subconfiguration σ_{x+E} there is a unique σ'_x such that $f(\sigma'_x|\sigma_{x+E}) = 1$. It is convenient to take the local neighborhood to be connected; this is no loss of generality since the amplitude vectors can be independent of part of the local configuration. In one dimension this means the local neighborhood is a sequence of k consecutive integers and local configurations can be written as strings $i_1 \ldots i_k$, $i_j \in Q$, indicating states of consecutive cells.

When any of the amplitude vectors has more than a single nonzero component the CA is called *indeterministic* [21]; probabilistic CA models for parallel computation, considered already in the original work of von Neumann and Ulam [22], fall into this class. Here we are interested in the quantum mechanical situation so the values of f are probability amplitudes and the state of the CA is described at each timestep by a *configuration vector* $\phi(t) \in \mathbb{C}L^Q$, the complex vector space with a basis $\{|\sigma\rangle \mid \sigma \in L^Q\}$ labelled by the configurations. The global evolution map $F : \mathbb{C}L^Q \to \mathbb{C}L^Q$ is defined on the configuration basis by

$$F|\sigma\rangle := \sum_{\sigma' \in L^Q} F_{\sigma'\sigma}|\sigma'\rangle, \tag{2.2a}$$

where

$$F_{\sigma'\sigma} := \prod_{x\in L} f(\sigma'_x|\sigma_{x+E}), \tag{2.2b}$$

and then extended linearly to all of the *configuration space* $\mathbb{C}L^Q$. Although the global evolution is linear on the configuration space, the local dynamics of the CA is *nonlinear* unless the local rule is constant or additive [23], *i.e.*, unless the amplitude vector is a linear function of the local configuration.

When the CA is deterministic, each factor in the product (2.2b) is either 0 or 1. If any is 0 the product is 0, otherwise it is 1. Thus definition (2.2) subsumes definition (2.1).

When the CA is indeterministic, however, we must be more precise about the meaning of the product in (2.2b). There are two possiblities:

If $L = \mathbb{Z}_N$ there is no problem. All the *transition amplitudes* $F_{\sigma'\sigma}$ are defined by finite products. To study the CA on an infinite lattice, we may take the usual statistical mechanics approach of computing some property (*e.g.*, a correlation function) on a sequence of lattices of increasing size and investigating the limiting behaviour of that property. With this methodology in mind we refer to a family of CAs $(\mathbb{Z}_N, Q, f, E)$ for all positive integers N as a *periodic* CA and call a configuration *admissible* for a periodic CA if it is periodic with any finite period N.

If $L = \mathbb{Z}$, the infinite product (2.2b) is defined as the limit of a sequence of partial products. A nonzero limit only exists if the successive factors in the product converge to 1. Since the range of f is at most q^{k+1} points in $\mathbb{C}$, this can only happen if beyond some stage all the factors in the product are 1. For any configuration σ define the *limit set*

$$\Omega^+(\sigma) := \{\lambda \in Q^k \mid \forall R > 0, \exists x > R : \sigma_{x+E} = \lambda\},$$

and define $\Omega^-(\sigma)$ similarly, *i.e.*, by conditioning on the existence of $x < -R$. We will refer to the two maximal semi-infinite subconfigurations of σ which contain only E-subconfigurations from the respective limit set as the *ends* of σ. Then σ has a nonzero transition amplitude to some configuration only if for each $\lambda \in \Omega^\pm(\sigma)$ some component of the amplitude vector $|\lambda\rangle\!\rangle$ is 1. For any local rule f, let

$$B_f := \{\lambda \in Q^k \mid \exists i \in Q : f(i|\lambda) = 1\},$$

be the set of local configurations with *big* amplitude vectors. This description is justified by the observation that for each $\lambda \in B_f$, the length of its amplitude vector is greater than or equal to 1. Call a set of configurations $A \subset \mathbb{Z}^Q$ *admissible* iff

(*i*) $\forall \sigma, \sigma' \in A$, $F_{\sigma'\sigma}$ is well defined.
(*ii*) $\forall \sigma \in A$, $\exists \sigma' \in A$ such that $F_{\sigma'\sigma} \neq 0$.
(*iii*) $\forall \sigma \in A$, $\sigma' \in \mathbb{Z}^Q$, if $F_{\sigma'\sigma} \neq 0$ then $\sigma' \in A$.

We allow *infinite* CAs only when the set of admissible configurations is nonempty. Several simple facts follow immediately:

LEMMA 2.1. *A is closed under the evolution. Furthermore, if $\sigma \in A$ then $\Omega^{\pm}(\sigma) \subset B_f$, and if $\Omega^{\pm}(\sigma') = \Omega^{\pm}(\sigma)$ then $\sigma' \in A$.*

The most familiar infinite CAs have a unique *quiescent* state [22], say 0, defined by the property that $f(i|0\ldots0) = \delta_{i0}$, *i.e.*, $B_f = \{0\ldots0\}$. (These are the only QCAs allowed in [12] and [18,19].) For such CAs admissible configurations have *finite support* in the sense that the only nonquiescent cells lie in some finite domain. It is clear that the collection of configurations with finite support is closed under the global evolution and, depending on f, may satisfy the admissibility conditions (i)–(iii); in Section 3 we show that these properties can hold for more interesting sets of configurations as well.

Consider the subspace of $\mathbb{C}L^Q$ with basis the admissible configurations A. This will become a Hilbert space, the *physical configuration space* H, once we define an inner product. Again using Dirac notation [20], but now for vectors $|\phi\rangle, |\psi\rangle \in \mathbb{C}A$ denoting states of a quantum system,

$$\langle\phi|\psi\rangle := \sum_{\sigma\in A} \overline{\phi}_\sigma \psi_\sigma,$$

where $|\phi\rangle = \sum_{\sigma\in A} \phi_\sigma|\sigma\rangle$ and similarly for $|\psi\rangle$. $H \subset \mathbb{C}A$ is the set of vectors with finite norm. A periodic or infinite CA is a *quantum* CA if the global evolution preserves this inner product and is time reversible (which is a distinct condition for infinite dimensional Hilbert space [24]), *i.e.*, is *unitary*. The physical interpretation is that when the system is described by the configuration vector $|\phi\rangle$ with $\langle\phi|\phi\rangle = 1$, the probability of observing it to be in configuration σ is $\overline{\phi}_\sigma\phi_\sigma$. The invariance of the inner product implies conservation of probability [20,24].

3. The unitarity constraints

The condition that the global evolution of a QCA be unitary places strict constraints on the local rule f. These constraints can be expressed directly in terms of the amplitude vectors:

THEOREM 3.1. *F is unitary iff for all admissible configurations σ' and σ'',*

$$\prod_{x\in L} \langle\!\langle \sigma''_{x+E} | \sigma'_{x+E} \rangle\!\rangle = \delta_{\sigma''\sigma'}, \tag{3.1}$$

and, in the infinite case, F is surjective.

Proof. F is unitary iff it preserves inner products and is surjective. For finite dimensional F the former condition implies the latter, as well as that $F^{-1} = F^\dagger$. In the infinite case both conditions are necessary and sufficient to reach this conclusion [25]. The condition that F preserves inner products is equivalent to $I = F^\dagger F$; in components this becomes:

$$\delta_{\sigma''\sigma'} = \sum_{\sigma\in A} (F^\dagger)_{\sigma''\sigma} F_{\sigma\sigma'} = \sum_{\sigma\in A} \overline{F}_{\sigma\sigma''} F_{\sigma\sigma'}$$

$$
\begin{aligned}
&= \sum_{\sigma\in A} \overline{\prod_{x\in L} f(\sigma_x|\sigma''_{x+E})} \prod_{y\in L} f(\sigma_y|\sigma'_{y+E}) \\
&= \sum_{\sigma\in A} \prod_{x\in L} \overline{f(\sigma_x|\sigma''_{x+E})} f(\sigma_x|\sigma'_{x+E}) \\
&= \cdots \sum_{\sigma_{x_i}\in Q} \cdots \prod_{x\in L} \overline{f(\sigma_x|\sigma''_{x+E})} f(\sigma_x|\sigma'_{x+E}),
\end{aligned}
$$

(where the ellipses denote sums for each $x_i \in L$ and by admissibility condition (*iii*), only $\sigma \in A$ make nonzero contributions)

$$
\begin{aligned}
&= \prod_{x\in L} \sum_{\sigma_x\in Q} \overline{f(\sigma_x|\sigma''_{x+E})} f(\sigma_x|\sigma'_{x+E}) \\
&= \prod_{x\in L} \langle\!\langle \sigma''_{x+E}|\sigma'_{x+E}\rangle\!\rangle,
\end{aligned}
$$

which is, of course, no more than the familiar condition for unitarity we described in [8] from the perspective of the sum-over-histories approach to quantum mechanics [26], written in terms of the transition amplitudes (2.2b). ■

A priori Theorem 3.1 tells us only that inner product invariance requires a constraint for each pair of admissible configurations. To be able to verify unitarity for arbitrarily large or infinite lattices given a local rule we must reduce the number to something independent of the cardinality of L. We do so in Subsections 3.1 and 3.2; then in Subsection 3.3 we consider the surjectivity condition which must also be satisfied for infinite lattices. Our results in this section are similar to those obtained independently by Dürr, Thanh and Santha [18,19].

3.1. The normalization constraints ...

There is one diagonal constraint in (3.1) for each admissible configuration:

$$
1 = \prod_{x\in L} \langle\!\langle \sigma_{x+E}|\sigma_{x+E}\rangle\!\rangle. \tag{3.2}
$$

That is, for each admissible configuration, the product of the lengths of the amplitude vectors of its E-subconfigurations must be 1. So to understand the structure of this set of constraints, we must understand which sets of E-subconfigurations can occur together. Since our configurations are one dimensional they may be constructed by appending (and prepending) one element of Q after another; each successive element is the right (left) most component of a corresponding E-subconfiguration which is determined by the new element together with the previous $k-1$ elements.

This construction may be realized by a *directed graph* (known as a de Bruijn graph [27]) which is weighted [28]: Let $G_1(Q,k)$ be the (q,q)-valent directed graph with vertices labelled by the elements of Q^{k-1} and directed edges labelled by $i_k \in Q$ connecting vertices labelled $i_1 i_2 \ldots i_{k-1}$ to vertices labelled $i_2 \ldots i_{k-1} i_k$. (See Figures 1 and 3 in Section 4 for

examples.) A *path* of length l in $G_1(Q,k)$ is a sequence of l directed edges in the graph, each of which (but the first) is directed away from the vertex to which the previous edge is directed. Paths of length l correspond bijectively to subconfigurations of length $l+k-1$; each edge corresponds to an E-subconfiguration.* A *cycle* in a directed graph is a closed path which passes through no vertex more than once.

Assign the weight $\langle\!\langle i_1 i_2 \ldots i_k | i_1 i_2 \ldots i_k \rangle\!\rangle$ to each edge labelled i_k leaving a vertex labelled $i_1 i_2 \ldots i_{k-1}$ and define the weight of a path in the directed graph to be the product of the weights of its edges. Then the weight of the path corresponding to configuration σ is given by the right hand side of (3.2).

LEMMA 3.2. *If (3.2) holds for every admissible configuration then the weight of every cycle in $G_1(Q,k)$ is 1.*

Proof. Since any cycle corresponds to an admissible configuration σ of a periodic CA for some N, (3.2) must hold for σ, proving the statement in the periodic case. In the infinite case, consider any cycle with edges labelled $i_1 \ldots i_l$ and a bi-infinite path in $G_1(Q,k)$ containing the cycle which corresponds to an admissible configuration σ. σ must have a subconfiguration corresponding to the cycle starting after some $x_0 \in \mathbb{Z}$: $\sigma_{x_0+j} = i_j$ for $1 \le j \le l$ and $\sigma_{x_0+l+j} = i_j$ for $0 \le j \le k-1$. Define a new configuration σ' by

$$\sigma'_x = \begin{cases} \sigma_x & \text{if } x \le x_0; \\ \sigma_{x+l} & \text{if } x > x_0. \end{cases}$$

$\Omega^{\pm}(\sigma') = \Omega^{\pm}(\sigma)$, so σ' is admissible by Lemma 2.1. Furthermore, the product in (3.2) will be identical for σ and σ' but for an extra product in the former of the weights of edges in the cycle. Since (3.2) holds for both σ and σ', the weight of the cycle must be 1. ■

THEOREM 3.3. *For a periodic CA, (3.2) holds for all admissible configurations iff the weight of every cycle in $G_1(Q,k)$ is 1.*

Proof. Lemma 3.2 is the 'only if' part of this statement. The 'if' part is almost a tautology since the only configurations in a periodic CA correspond to collections of cycles, so if each has weight 1, then (3.2) holds for all admissible configurations. ■

The analogous result in the infinite case is somewhat more complicated because the admissible configurations are different. Let us examine them more closely:

LEMMA 3.4. *Let σ be any configuration in an infinite CA. Then $\Omega^{\pm}(\sigma)$ consists of E-subconfigurations corresponding to the edges in a collection of cycles in $G_1(Q,k)$.*

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* Equivalently, $G_1(Q,k)$ is a *finite state automaton* (FSA; see, *e.g.*, [29]) with states corresponding to length $k-1$ subconfigurations and transitions to single elements of Q. Such FSAs model circuits with memory, like convolutional coders [30]. When the outputs of an FSA are (state,transition) pairs it is called a *Mealy machine* [31]; here the outputs are E-subconfigurations.

Proof. We must show that for any E-subconfiguration $\lambda \in \Omega^+(\sigma)$ there is some cycle in $G_1(Q,k)$ containing the edge corresponding to λ such that the E-subconfiguration corresponding to each edge in the cycle is also in $\Omega^+(\sigma)$. By definition, $\lambda \in \Omega^+(\sigma)$ only if the corresponding edge in $G_1(Q,k)$ is traversed infinitely many times by the infinite forward path corresponding to σ. To return to this edge the infinite forward path must contain a cycle; to return to it infinitely many times it must contain at least one of the only finitely many cycles infinitely many times. Each edge in that cycle is therefore traversed infinitely many times by the infinite forward path corresponding to σ and hence the corresponding E-subconfigurations are in $\Omega^+(\sigma)$. The analogous proof with 'forward' replaced by 'backward' proves the statement for $\Omega^-(\sigma)$. ■

Applying Lemma 2.1, we have the immediate:

COROLLARY 3.5. *An infinite CA has admissible configurations only if there is a subset $D_f \subset B_f$ of local configurations corresponding to the edges in a collection of cycles of $G_1(Q,k)$.*

Let $D_1(Q,k,f)$ be the subgraph of $G_1(Q,k)$ consisting of these cycles. A maximal D_f which is closed under the evolution will be referred to as the *deterministic sector* of a QCA because of the following result:

THEOREM 3.6. *If F is unitary then when restricted to local configurations in D_f, the local rule is deterministic. If D_f is closed under the evolution then the set of configurations defined by $A := \{\sigma \mid \Omega^{\pm}(\sigma) \subset D_f\}$ is admissible.*

Proof. By Corollary 3.5, each $\lambda \in D_f \subset B_f$ corresponds to an edge in a $G_1(Q,k)$ cycle, each edge of which corresponds to a local configuration $\lambda_i \in D_f$, $1 \le i \le l$. By Theorem 3.1 and Lemma 3.2, if F is unitary,

$$1 = \prod_{i=1}^{l} \langle\langle \lambda_i | \lambda_i \rangle\rangle. \tag{3.3}$$

When we defined B_f we observed that for each $\lambda \in B_f$, $|\lambda\rangle\rangle$ has norm at least 1; now (3.3) implies that each λ_i in this cycle, and hence every local configuration in D_f, has an amplitude vector with norm exactly 1. Since each amplitude vector has at least one component equal to 1, all the remaining components must be 0; thus the local rule is deterministic.

Since F restricted to local configurations in D_f is deterministic, for any $\sigma, \sigma' \in A$, either the ends of σ evolve to those of σ', in which case $F_{\sigma'\sigma}$ is well defined; or they do not, in which case $F_{\sigma'\sigma} = 0$, which is still well defined. This verifies admissibility condition (i). Furthermore, D_f is closed under the evolution means that for every path of length k in D_f, corresponding to a subconfiguration $i_1 \ldots i_{2k-1}$, the unique local configuration $i'_1 \ldots i'_k$ defined by $f(i'_j | i_j \ldots i_{j+k-1}) = 1$, $1 \le j \le k$, corresponds to an edge in D_f. If F is unitary then it is norm preserving, so for any $\sigma \in A$, there must be some $\sigma' \in \mathbb{Z}^Q$ with $F_{\sigma'\sigma} \ne 0$.

Since D_f is closed under the evolution, $\Omega^{\pm}(\sigma') \subset D_f$; this verifies admissibility conditions (ii) and, since D_f is maximal, (iii). ∎

Since we only consider infinite CAs with admissible configurations, we will assume henceforth that each has a nonempty deterministic sector which defines the set of admissible configurations as in Theorem 3.6. The remarkable consequence of this theorem is that an infinite QCA must be *asymptotically deterministic*: the only admissible configurations are those which evolve deterministically outside some finite domain. Indeterministic quantum evolution can only occur for a finite subconfiguration interpolating between the ends of the configuration. Thus the analogue of Theorem 3.3 for infinite CAs is:

THEOREM 3.7. *For an infinite CA, (3.2) holds for all admissible configurations iff the weight of every cycle in $G_1(Q,k)$ is 1 and the weight of every acyclic path in $G_1(Q,k)$ terminating at vertices in $D_1(Q,k,f)$ is 1.*

Proof. By Lemma 3.2, if (3.2) holds for all admissible configurations then the weight of every cycle in $G_1(Q,k)$ is 1. Consider any acyclic path connecting cycles in $D_1(Q,k,f)$. By Theorem 3.6, there is an admissible configuration corresponding to a bi-infinite path contained in $D_1(Q,k,f)$ except for a finite segment along the chosen acyclic path. If (3.2) holds for all admissible configurations the weight of the whole path is 1, as are the weights of the two ends in $D_1(Q,k,f)$; hence the weight of the acyclic path is also 1. Conversely, by definition and by Lemma 3.4, the only admissible configurations are those with ends corresponding to collections of cycles, connected by a finite subconfiguration which, after removing some finite number of subconfigurations corresponding also to cycles in $G_1(Q,k)$, is an acyclic path terminating at vertices in $D_1(Q,k,f)$. If all the cycles and the acyclic path have weight 1 then (3.2) holds. ∎

3.2. ... and the orthogonality constraints

There is one off-diagonal constraint in (3.1) for each pair of distinct admissible configurations:

$$0 = \prod_{x\in L} \langle\!\langle \sigma''_{x+E} | \sigma'_{x+E} \rangle\!\rangle. \tag{3.4}$$

By (3.2), for each x such that $\sigma''_{x+E} = \sigma'_{x+E}$, the corresponding factor in (3.4) is nonzero. Thus at least one of the pairs of *mismatched* E-subconfigurations $\sigma''_{x+E} \neq \sigma'_{x+E}$ must contribute a factor of 0 in order for the product in (3.4) to vanish. To understand this set of orthogonality constraints, therefore, we must understand which sets of pairs of mismatched E-subconfigurations can occur together. We construct a new weighted directed graph which generates these sets:

Let $G_2(Q,k)$ be the (q^2,q^2)-directed graph with vertices labelled by the elements of $Q^{k-1}\times Q^{k-1}$ and directed edges labelled by $(i''_k, i'_k) \in Q^2$ connecting vertices labelled $(i''_1 i''_2 \ldots i''_{k-1}, i'_1 i'_2 \ldots i'_{k-1})$ to vertices labelled $(i''_2 \ldots i''_{k-1} i''_k, i'_2 \ldots i'_{k-1} i'_k)$. Note that there is a subgraph of $G_2(Q,k)$ isomorphic to $G_1(Q,k)$, namely those vertices and edges with both components of these labels identical; so we write $G_1(Q,k) \subset G_2(Q,k)$. (See Figure 2

in Section 4 for an example.)

Paths in $G_2(Q,k)$ correspond bijectively to *pairs* of subconfigurations; each edge corresponds to a pair of E-subconfigurations. We assign the weight $\langle\!\langle i''_1 i''_2 \ldots i''_k | i'_1 i'_2 \ldots i'_k \rangle\!\rangle$ to each edge labelled (i''_k, i'_k) leaving a vertex labelled $(i''_1 i''_2 \ldots i''_{k-1}, i'_1 i'_2 \ldots i'_{k-1})$ so that the weight of the path corresponding to a pair of configurations σ' and σ'' is given by the right hand side of (3.4). Two configurations σ' and σ'' are distinct only if they have at least one pair of mismatched E-subconfigurations, so a path in $G_2(Q,k)$ corresponds to them only if it intersects $M(Q,k) := G_2(Q,k) \setminus G_1(Q,k)$.

LEMMA 3.8. *If F is unitary then the weight of every acyclic path in $M(Q,k)$ terminating at vertices of $G_1(Q,k)$ is 0.*

Proof. Any acyclic path in $M(Q,k)$ terminating at vertices of $G_1(Q,k)$ can be extended, using only edges in $G_1(Q,k)$, to a path in $G_2(Q,k)$ corresponding to a pair of distinct admissible configurations σ' and σ''. If F is unitary, however, Theorem 3.1 implies condition (3.2), which precludes the weight of any edge in $G_1(Q,k)$ from vanishing. Thus (3.4) can only be satisfied for σ' and σ'' if the weight of the portion of the path in $M(Q,k)$ vanishes. ∎

THEOREM 3.9. *For a periodic CA, F is unitary iff all of the following are true:*

(i) The weight of every cycle in $G_1(Q,k)$ is 1.
(ii) The weight of every cycle in $M(Q,k)$ is 0.
(iii) The weight of every acyclic path in $M(Q,k)$ terminating at vertices in $G_1(Q,k)$ is 0.

Proof. If F is unitary then Theorem 3.1 and Lemma 3.2 imply (i) while Theorem 3.1 and Lemma 3.8 imply (iii). Any cycle in $M(Q,k)$ corresponds to a pair of distinct admissible configurations σ' and σ'' of a periodic CA for some N. Theorem 3.1 implies (3.4) must hold for σ' and σ''; this implies (ii).

Conversely, by Theorem 3.3, (i) implies (3.2) holds for all admissible configurations in a periodic CA. Furthermore, pairs of distinct admissible configurations in a periodic CA correspond to collections of cycles in $G_2(Q,k)$, at least one of which intersects $M(Q,k)$. Thus (3.4) holds if each cycle which intersects $M(Q,k)$ has weight 0; (ii) and (iii) imply that this is the case. By Theorem 3.1, (3.2) and (3.4) imply F is unitary. ∎

Before stating the analogous result in the infinite case, we define $D_2(Q,k,f)$ to be the subgraph of $G_2(Q,k)$ consisting of the edges corresponding to pairs of local configurations each of which is in D_f.

THEOREM 3.10. *For an infinite CA, F is unitary iff all of the following are true:*

(i) The weight of every cycle in $G_1(Q,k)$ is 1.
(ii) The weight of every acyclic path in $G_1(Q,k)$ terminating at vertices in $D_1(Q,k,f)$ is 1.
(iii) The weight of every acyclic path in $M(Q,k)$ terminating at vertices in $G_1(Q,k)$ is 0.

(iv) The weight of every cycle in $D_2(Q,k,f) \cap M(Q,k)$ is 0.
(v) F is surjective.

Proof. If F is unitary then Theorem 3.1 and Theorem 3.7 imply (i), (ii) and (v), while Theorem 3.1 and Lemma 3.8 imply (iii). Any cycle in $D_2(Q,k,f) \cap M(Q,k)$ can be repeated infinitely and then corresponds to a pair of distinct admissible configurations σ' and σ'' (since the ends of each are contained in D_f). Theorem 3.1 implies (3.4) must hold for σ' and σ''; this implies (iv).

Conversely, by Theorem 3.7, (i) and (ii) imply (3.2) holds for all admissible configurations in an infinite CA. Furthermore, pairs of distinct admissible configurations in an infinite CA correspond to bi-infinite paths in $G_2(Q,k)$ which consist of cycles in $D_2(Q,k,f)$ at both ends. If any one of these cycles lies in $D_2(Q,k,f) \cap M(Q,k)$ then (iv) implies (3.4) holds. If none of the cycles contains only edges corresponding to mismatched E-subconfigurations then there must be an acyclic path in $M(Q,k)$ terminating at vertices in $G_1(Q,k)$. In this case (iii) implies (3.4) holds. By Theorem 3.1, (v), (3.2) and (3.4) imply F is unitary. ■

3.3. Surjectivity

To complete the program of determining a collection of constraints on the amplitude vectors which is equivalent to unitarity of the global evolution we must show that for infinite CAs, condition (v) of Theorem 3.10—surjectivity—is equivalent to some collection of such constraints.

By Theorem 3.6 each $\sigma \in A$ has a minimal length *interior* subconfiguration $I(\sigma) = \sigma_{x_0+1} \ldots \sigma_{x_0+n}$, defined by the condition that if $j < x_0 + 1$ or $j > x_0 + n + k - 1$ then $\sigma_{j-k+1} \ldots \sigma_j \in \Omega^{\pm}(\sigma)$, respectively. We will refer to the semi-infinite subconfigurations $\ldots \sigma_{x_0}$ and $\sigma_{x_0+n+1} \ldots$ as the *deterministic ends* of σ. For example, if $D_f = \{000, 111\}$ ($k = 3$) then a possible admissible configuration is $\sigma = \ldots 0\sigma_1 \ldots \sigma_n 1 \ldots$ and $I(\sigma) = \sigma_1 \ldots \sigma_n$, provided $\sigma_1 \neq 0$ and $\sigma_n \neq 1$. Let $A_n := \{\sigma \in A \mid |I(\sigma)| = n\}$. Then $A = \cup A_n$, $0 \leq n < \infty$. We will find a necessary and sufficient set of constraints on f such that F maps onto A_n for each nonnegative integer n; since A is an orthonormal basis for H this is equivalent to F mapping onto H.

We begin by observing that F already maps onto the *completely deterministic configurations* A_0. More precisely,

LEMMA 3.11. *For an infinite CA, if F is norm preserving (i.e., if conditions (i)—(iv) of Theorem 3.10 hold) then $F : A_0 \to A_0$ is surjective.*

Proof. If F is norm preserving it is injective on $H \supset A_0$. By definition, all E-subconfigurations of A_0 are in D_f, so F is deterministic on A_0.* Every configuration $\sigma \in A_0$ corresponds

* Notice that neither Moore and Myhill's Garden of Eden Theorem [32] nor Hedlund's result that injectivity implies surjectivity for endomorphisms of shift dynamical systems [33] may be applied to

to a sequence of cycles in $D_1(Q,k,f)$ since $I(\sigma)=\emptyset$. But injectivity implies surjectivity for F restricted to cycles in $D_1(Q,k,f)$: Each cycle of length m must map to a closed path of length m which, by injectivity, must also be a cycle. There are only a finite number of length m cycles and by injectivity F maps no two to the same one; hence F is surjective on cycles in $D_1(Q,k,f)$. ■

This result has an immediate corollary once we make some suitable definitions:

COROLLARY 3.12. *For an infinite CA, if F is norm preserving then the restriction of F to semi-infinite completely deterministic admissible subconfigurations is surjective.*

To define the restriction of F on subconfigurations it will be convenient in the rest of this subsection to take neighborhoods of size k to be defined by $E:=\{0,\ldots,k-1\}$. Any other connected local neighborhood of the same size is equivalent to this choice after a translation, so there is no loss of generality. Having made this choice for E, we may define the restriction of F to any subconfiguration $\sigma_a\ldots\sigma_b$ of any admissible configuration by

$$F|\sigma_a\ldots\sigma_b\rangle := \sum_{\sigma'_a\ldots\sigma'_{b-k+1}} |\sigma'_a\ldots\sigma'_{b-k+1}\rangle \prod_{i=a}^{b-k+1} f(\sigma'_i|\sigma_i\ldots\sigma_{i+k-1}), \tag{3.5}$$

which is well defined even when either $a=-\infty$ or $b=\infty$ since $\sigma_a\ldots\sigma_b$ is a subconfiguration of an admissible configuration. ((3.5) is equivalent to (2.2a,b) when $a=-\infty, b=\infty$.) Now we can prove Corollary 3.12:

Proof. By definition, a semi-infinite completely deterministic admissible subconfiguration is a deterministic end of at least one configuration in A_0. By Lemma 3.11, F is surjective on A_0; whence the restriction of F defined by (3.5) to subconfigurations of configurations in A_0 is also surjective. ■

This means that F restricted to the deterministic ends of admissible configurations is surjective and indicates that we may concentrate just on interior subconfigurations. For $\lambda=\lambda_0\ldots\lambda_{k-1}$, $\rho=\rho_0\ldots\rho_{k-1}\in D_f$ define

$$\begin{aligned} A_n^{(\rho)} &:= \{i_1\ldots i_n\rho_0\ldots\rho_{k-2} \mid i_j\in Q, 1\le j\le n\} \\ A_n^{(\lambda,\rho)} &:= \{\lambda_1\ldots\lambda_{k-1}i_1\ldots i_n\rho_0\ldots\rho_{k-2} \mid i_j\in Q, 1\le j\le n\}. \end{aligned}$$

Considering an element of $A_n^{(\lambda,\rho)}$ to be a subconfiguration of an admissible configuration we may use (3.5) to define the action of F on $A_n^{(\lambda,\rho)}$.

THEOREM 3.13. *For an infinite CA with F norm preserving, F maps onto A_n for $0<n\in\mathbb{Z}$ iff for all $\lambda,\rho'\in D_f$, its restriction $F_n^{(\lambda,\rho')}: A_n^{(\lambda,\rho)}\to A_n^{(\rho')}$ is surjective when $f(\rho'_{k-1}|\rho)=1$.*

conclude that F is surjective on A_0 since A, and hence A_0, is only a proper subset of the set of all possible configurations.

Proof. Each configuration $\sigma' \in A_n$ has an interior subconfiguration of length n extended by deterministic ends: $\sigma' = \ldots \lambda'_{k-1} i'_1 \ldots i'_n \rho'_0 \ldots$ where $\sigma'_{x_0} = i'_1$, say, and $\lambda'_{j-k+1} \ldots \lambda'_j \in D_f$ for $j \le k-1$, $\rho'_j \ldots \rho'_{j+k-1} \in D_f$ for $j \ge 0$. F maps onto A_n iff for all $\sigma' \in A_n$,

$$|\sigma'\rangle = F \sum c_m |\sigma^m\rangle \tag{3.6}$$

for some element $\sum c_m |\sigma^m\rangle \in H$. By Corollary 3.12, there exist semi-infinite deterministic configurations $\ldots \lambda_{k-1}$ and $\rho_0 \ldots$ such that $\langle \sigma' | F | \sigma^m \rangle \ne 0$ only for configurations of the form $\sigma^m = \ldots \lambda_0 \ldots \lambda_{k-1} i^m_1 \ldots i^m_n \rho_0 \ldots$, where $\sigma_{x_0} = \lambda_1$ and

$$\begin{aligned} F|\ldots\lambda_0\ldots\lambda_{k-1}\rangle &= |\ldots\lambda'_{k-1}\rangle \\ F|\rho_0\ldots\rangle &= |\rho'_0\ldots\rangle. \end{aligned} \tag{3.7}$$

For these configurations (3.5) implies that

$$\langle \sigma' | F | \sigma^m \rangle = \langle i'_1 \ldots i'_n \rho'_0 \ldots \rho'_{k-2} | F | \lambda_1 \ldots \lambda_{k-1} i^m_1 \ldots i^m_n \rho_0 \ldots \rho_{k-2} \rangle. \tag{3.8}$$

Combining (3.6), (3.7) and (3.8) we find

$$|i'_1 \ldots i'_n \rho'_0 \ldots \rho'_{k-2}\rangle = F \sum c_m |\lambda_1 \ldots \lambda_{k-1} i^m_1 \ldots i^m_n \rho_0 \ldots \rho_{k-2}\rangle, \tag{3.9}$$

which is exactly the statement that $F_n^{(\lambda,\rho')}$ is surjective. Since $\lambda' := \lambda'_0 \ldots \lambda'_{k-1} \in D_f$ is arbitrary and $f(\lambda'_{k-1}|\lambda) = 1$ (from (3.7)) defines a unique $\lambda := \lambda_0 \ldots \lambda_{k-1} \in D_f$ by Corollary 3.12, λ is an arbitrary deterministic local configuration. Furthermore, (3.7) implies $f(\rho'_{k-1}|\rho) = 1$ for $\rho := \rho_0 \ldots \rho_{k-1}$; this completes the "only if" direction of the proof. Conversely, if for all $\lambda, \rho' \in D_f$ with $f(\rho'_{k-1}|\rho) = 1$, (3.9) holds for some $c_m \in \mathbb{C}$, then using Corollary 3.12 we can construct arbitrary deterministic ends satisfying (3.7) and conclude that (3.6) holds for all $\sigma' \in A_n$. ■

With Lemma 3.11 and Theorem 3.13 we have reduced the problem of the surjectivity of the infinite dimensional map F to the equivalent problem of the surjectivity of the finite dimensional maps F_n for all $1 \le n \in \mathbb{Z}$ (we will supress the superscripts (λ, ρ') in the following). But F_n is onto iff $\det F_n \ne 0$. To understand these conditions we must explicate the structure of F_n. Notice first that as an immediate consequence of definition (3.5) each column of F_n has a common factor. More precisely,

LEMMA 3.14. *For $\alpha, \alpha' \in Q^n$,*

$$(F_n)_{\alpha',\alpha} = (\tilde{F}_n)_{\alpha',\alpha} \cdot \begin{cases} \langle \rho'_0 \ldots \rho'_{k-2} | F | \alpha_{n-k+2} \ldots \alpha_n \rho_0 \ldots \rho_{k-2} \rangle, & \text{if } n \ge k-1; \\ \langle \rho'_0 \ldots \rho'_{k-2} | F | \lambda_{n+1} \ldots \lambda_{k-1} \alpha \rho_0 \ldots \rho_{k-2} \rangle, & \text{if } 0 \le n < k-1; \end{cases} \tag{3.10}$$

where $\tilde{F}$ is the reduced transition matrix *defined by*

$$(\tilde{F}_n)_{\alpha',\alpha} := \langle \alpha' | F | \lambda_1 \ldots \lambda_{k-1} \alpha \rangle. \tag{3.11}$$

These common factors can be pulled out of each column in the determinant:

COROLLARY 3.15. $\det F_n = c_n \det \tilde{F}_n$, *where*

$$c_n := \begin{cases} \prod_{\gamma\in Q^{k-1}} \langle \rho'_0 \ldots \rho'_{k-2}|F|\gamma\rho_0\ldots\rho_{k-2}\rangle^{q^{n-k+1}}, & \text{if } n \geq k-1; \\ \prod_{\alpha\in Q^n} \langle \rho'_0 \ldots \rho'_{k-2}|F|\lambda_{n+1}\ldots\lambda_{k-1}\alpha\rho_0\ldots\rho_{k-2}\rangle, & \text{if } 0 \leq n < k-1. \end{cases} \tag{3.12}$$

Proof. When $n \geq k-1$, for each $\gamma \in Q^{k-1}$ there are q^{n-k+1} columns in F_n labelled by subconfigurations having γ as their last $k-1$ states. According to Lemma 3.14, the factor in (3.10) occurs in each. When $0 \leq n < k-1$, for each $\alpha \in Q^n$ there is exactly one column in F_n labelled by α. Again, by Lemma 3.14, this column contains the factor in (3.10). ■

Second, for $\gamma \in Q^{k-1}$, let

$$\Phi^{(\gamma)} := \begin{pmatrix} |\gamma 0\rangle\rangle \\ \vdots \\ |\gamma(q-1)\rangle\rangle \end{pmatrix} \in M_q(\mathbb{C}). \tag{3.13}$$

Now we can find a recurrence relation (with initial condition $\tilde{F}_0 = 1$) for the reduced transition matrix:

LEMMA 3.16. *$\tilde{F}_{n+1}$ can be expressed in terms of $\tilde{F}_n$ and the $\Phi^{(\gamma)}$ as*

$$(\tilde{F}_{n+1})_{\alpha' j,\alpha i} = (\tilde{F}_n)_{\alpha',\alpha} \cdot \begin{cases} \Phi_{ij}^{(\alpha_{n-k+2}\ldots\alpha_n)}, & \text{if } n \geq k-1; \\ \Phi_{ij}^{(\lambda_{n+1}\ldots\lambda_{k-1}\alpha)}, & \text{if } 0 \leq n < k-1; \end{cases} \tag{3.14}$$

where $\alpha, \alpha' \in Q^n$ and $i, j \in Q$.

Proof. Apply definition (3.11):

$$\begin{aligned} (\tilde{F}_{n+1})_{\alpha' j,\alpha i} &= \langle \alpha' j|F|\lambda_1\ldots\lambda_{k-1}\alpha i\rangle \\ &= \langle \alpha'|F|\lambda_1\ldots\lambda_{k-1}\alpha\rangle \cdot \begin{cases} f(j|\alpha_{n-k+2}\ldots\alpha_n i), & \text{if } n \geq k-1; \\ f(j|\lambda_{n+1}\ldots\lambda_{k-1}\alpha i), & \text{if } 0 \leq n < k-1; \end{cases} \end{aligned}$$

where the second equality follows from definition (3.5). Definition (3.13) gives the result (3.14). ■

Just as the common factors in Lemma 3.14 could be pulled out of the determinant of F_n in Corollary 3.15, so too can the *determininants* of the common tensor factors $\Phi^{(\gamma)}$. We need two simple properties of determinants:

1. For $i, j \in \{1, \ldots, m\}$, let $X_{ij} \in M_n(\mathbb{C})$ be $m \times m$ matrices over $\mathbb{C}$. Suppose $X_{i1} = x_i B$ with $x_i \in \mathbb{C}$ and $B \in M_n(\mathbb{C})$. Then

$$\det \begin{pmatrix} X_{11} & \cdots & X_{1m} \\ \vdots & & \vdots \\ X_{m1} & \cdots & X_{mm} \end{pmatrix} = \det B \det \begin{pmatrix} x_1 I & X_{12} & \cdots & X_{1m} \\ \vdots & \vdots & & \vdots \\ x_m I & X_{m2} & \cdots & X_{mm} \end{pmatrix}, \tag{3.15}$$

   for I the $n \times n$ identity matrix.

2. Let $X \in M_m(\mathbb{C})$. Then

$$\det(X \otimes I) = (\det X)^n \tag{3.16}$$

   where I is again the $n \times n$ identity matrix.

COROLLARY 3.17. $\det \tilde{F}_{n+1} = d_{n+1}[\det \tilde{F}_n]^q$, *where*

$$d_{n+1} := \begin{cases} \prod_{\gamma \in Q^{k-1}} [\det \Phi^{(\gamma)}]^{q^{n-k+1}}, & \text{if } n \geq k-1; \\ \prod_{\alpha \in Q^n} \det \Phi^{(\lambda_{n+1} \ldots \lambda_{k-1} \alpha)}, & \text{if } 0 \leq n < k-1. \end{cases} \tag{3.17}$$

Proof. By Lemma 3.16 the columns of $\tilde{F}_{n+1}$ come from the columns of $\tilde{F}_n$ tensored with the corresponding $\Phi^{(\gamma)}$. Applying (3.15) we have:

$$\det \tilde{F}_{n+1} = \det \tilde{F}_n \otimes I \cdot \begin{cases} \prod_{\gamma \in Q^{k-1}} [\det \Phi^{(\gamma)}]^{q^{n-k+1}}, & \text{if } n \geq k-1; \\ \prod_{\alpha \in Q^n} \det \Phi^{(\lambda_{n+1} \ldots \lambda_{k-1} \alpha)}, & \text{if } 0 \leq n < k-1 \end{cases}$$

(where I is the $q \times q$ identity matrix), by exactly the same reasoning as in the proof of Corollary 3.15, but now using the result of Lemma 3.16 for the common tensored matrices. Applying (3.16) gives the result (3.17). ∎

Putting these results together gives the Surjectivity Theorem summarizing the conditions that for all $1 \leq n \in \mathbb{Z}$, $\det F_n \neq 0$:

THEOREM 3.18. *An infinite CA with norm preserving F and deterministic sector D_f is surjective iff for all $\lambda, \rho, \rho' \in D_f$ such that $f(\rho'_{k-1}|\rho) = 1$, none of the following vanish:*

(i) $\langle \rho'_0 \ldots \rho'_{k-2} | F | \gamma \rho_0 \ldots \rho_{k-2} \rangle$
(ii) $\det \Phi^{(\gamma)}$

for any $\gamma \in Q^{k-1}$, $0 \leq n < k-1$.

Proof. By Corollaries 3.15 and 3.17, $\det F_n \neq 0$ for all $n \geq 0$ iff none of the c_n defined in (3.12) nor the d_n defined in (3.17) vanish. This is ensured by (*i*) and (*ii*), respectively, since

$$\{|\lambda_{n+1} \ldots \lambda_{k-1} \alpha \rho_0 \ldots \rho_{k-2}\rangle \mid \alpha \in Q^n, 0 \leq n < k-1\} \subset \{|\gamma \rho_0 \ldots \rho_{k-2}\rangle \mid \gamma \in Q^{k-1}\}$$

and

$$\{\Phi^{(\lambda_{n+1}\ldots\lambda_{k-1}\alpha)} \mid \alpha \in Q^n, 0 \leq n < k-1\} \subset \{\Phi^{(\gamma)} \mid \gamma \in Q^{k-1}\}.$$

■

We will refer to the nonvanishing of the expressions in (i) and (ii) as the *surjectivity constraints*. Each is a closed condition, so as we will see in the next section, when they are not inconsistent with constraints (i)–(iv) of Theorem 3.10, they do not reduce the dimension of the solution space.

4. Solutions

Theorems 3.9 and 3.10, to which we will refer as the Unitarity Theorems, and Surjectivity Theorem 3.18, together with the finiteness of the graph $G_2(Q,k)$, show that given a local rule f we can determine, by checking only a finite number of conditions, whether the global evolution is unitary, *i.e.*, whether f defines a QCA. This proves:

THEOREM 4.1. *Unitarity is decidable for 1 dimensional CAs.*

As yet we have no proposed local rule f for which to check unitarity. In the next two subsections we write down the constraints resulting from the Unitarity Theorems for binary (*i.e.*, $q = 2$) CAs in the two simplest cases and show that they can be solved to give multiparameter families of QCAs.

Before doing so, however, it is useful to discuss some symmetries of QCAs. First, note that the symmetry group of a one dimensional lattice L has two generators: T, translation by one and P, reflection in the origin/parity reversal. P acts on local configurations, sending $\lambda = i_1 \ldots i_k$ to $P\lambda = i_k \ldots i_1$. (To be precise, this is the case when k is odd; when k is even this transformation is TP if the origin is taken to be at the $\lfloor k/2 \rfloor$ position in the local neighborhood. It will cause no confusion, however, to denote both by P.) P may be defined to act on a local rule f by: $(Pf)(i|\lambda) := f(i|P\lambda)$; hence $P|i_1 \ldots i_k\rangle\!\rangle := |i_k \ldots i_1\rangle\!\rangle$. We will refer to Pf as the *parity transform* of f. Since $P^2 f = f$, any local rule which is not *symmetric*, *i.e.*, invariant under this reflection, will pair with a distinct parity transformed local rule.

Second, note that the symmetric group S_q acts on the set of states Q of a QCA. For $q = 2$ the symmetric group is generated by the transposition τ which interchanges 0 and 1.* τ acts on a local configuration $\lambda = i_1 \ldots i_k$ to give $\tau\lambda = \tau i_1 \ldots \tau i_k$, so it acts on a local rule in two ways:

$$(\tau_{\text{in}} f)(i|\lambda) := f(i|\tau\lambda)$$
$$(\tau_{\text{out}} f)(i|\lambda) := f(\tau i|\lambda).$$

These transformations will be most useful in the discussion of infinite, and hence asymptotically deterministic, QCAs.

* From a more physical perspective, τ is analogous to charge conjugation.

4.1. $k = 2$

The simplest nontrivial binary CAs have local neighborhoods of size 2.* Figure 1 shows G_1. (The arguments $Q = \{0,1\}$ and $k = 2$ are suppressed in this subsection.) Here all the relevant paths can be identified by inspection. More formally, define the transfer matrix A_1 for G_1 to be the 2×2 matrix with ij^{th} entry the weight of the edge from vertex i to vertex j:

$$A_1 = \begin{pmatrix} w_0 & w_1 \\ w_2 & w_3 \end{pmatrix},$$

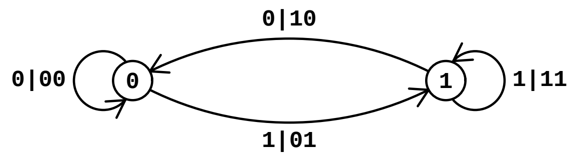

Figure 1. G_1 for binary CAs with local neighborhoods of size 2. Each vertex and edge is labelled, the latter by the number to the left of the slash. The weight of each edge is the squared norm of the amplitude vector of the local configuration indicated to the right of the slash.

where $w_\alpha := \langle\!\langle \alpha | \alpha \rangle\!\rangle$ and α is the base 10 (say) representation of the local configuration bit string. The ij^{th} entry in A_1^n is the sum of the weights of the paths with n edges from vertex i to vertex j, so it is useful to define the generating function

$$A_1(t) := \sum_{n \geq 0} A_1^n t^n.$$

The i^{th} diagonal entry in $A_1(t)$ is the sum of the weights of the paths of length n beginning and ending at vertex i, times t^n, for all $n \geq 0$; hence $\mathrm{Tr}A_1(t)$ is the corresponding sum over all closed paths in G_1. It is straightforward to show [28] that if $Z(t) := \det(I - tA)$ then

$$\mathrm{Tr}A(t) = -\frac{tZ'(t)}{Z(t)}. \tag{4.1}$$

Evaluating the righthand side of (4.1) for A_1 we find

$$\mathrm{Tr}A_1(t) = \frac{(w_0 + w_3 + 2w_1w_2t)t - 2w_0w_3t^2}{1 - (w_0 + w_3 + w_1w_2t)t + w_0w_3t^2}. \tag{4.2}$$

We can read off the weights of the cycles in G_1 directly from the positive terms in the numerator and the negative terms in the denominator of (4.2): w_0, w_3, and w_1w_2. (That these are the right terms becomes clear upon expanding (4.2) in powers of t:

$$\mathrm{Tr}A_1(t) = (w_0 + w_3)t + (2w_1w_2 - 2w_0w_3 + w_0^2 + 2w_0w_3 + w_3^2)t^2 + O(t^3),$$

where the cancelling coefficients of t^2 have been included to indicate the function of the other terms in (4.2).) This is more machinery than we need to find the cycles in G_1, of course, but it will become useful in more complicated situations.

* These are sometimes called 'one-way' automata [15] since the local neighborhood of x extends only to one side, although Hillman has pointed out that this terminology is somewhat misleading [34].

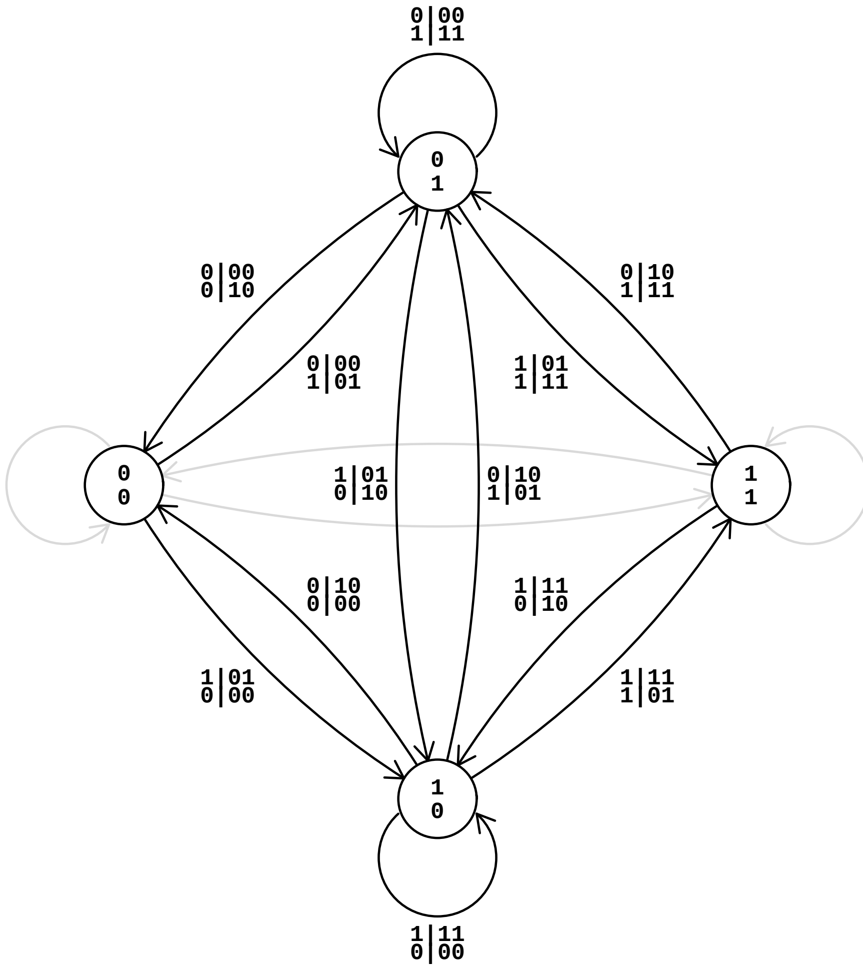

Figure 2. G_2 for binary CAs with local neighborhoods of size 2. The edges in the subgraph isomorphic to G_1 are grey and unlabelled; each other edge is labelled by the pair of numbers to the left of the slash and weighted by the inner product of the pair of amplitude vectors of the two local configurations to the right of the slash.

For either a periodic or an infinite QCA, each of these cycles must have weight 1—this is condition (i) in the Unitarity Theorems. Thus

$$1 = w_0 \tag{4.3a}$$

$$1 = w_3 \tag{4.3b}$$

$$1 = w_1 w_2. \tag{4.3c}$$

That is, both $|00\rangle\!\rangle$ and $|11\rangle\!\rangle$ must have norm 1, while $\langle\!\langle 10|10\rangle\!\rangle = \langle\!\langle 01|01\rangle\!\rangle^{-1}$.

Figure 2 shows G_2 with only the edges in M labelled and weighted; the subgraph isomorphic to G_1 is indicated with grey unlabelled edges. Since the orthogonality constraints are determined by the weights of paths in M, to simplify the transfer matrix we may set the weights of the edges from vertex $(0,0)$ to itself and from vertex $(1,1)$ to itself to 0 and

the weights of the edges between these two vertices to 1. Then

$$A_2 = \begin{pmatrix} 0 & w_{01} & w_{01} & 1 \\ w_{02} & w_{03} & w_{12} & w_{13} \\ w_{02} & w_{12} & w_{03} & w_{13} \\ 1 & w_{23} & w_{23} & 0 \end{pmatrix}, \tag{4.4}$$

where $w_{\alpha\beta} := \langle\!\langle\alpha|\beta\rangle\!\rangle$ and α,β are again base 10 (say) representations of the local configuration bit strings. Now,

$$\begin{aligned} Z_2(t) &:= \det(I - tA_2) \\ &= 1 - 2w_{03}t + (-1 - 2w_{01}w_{02} + w_{03}^2 - w_{12}^2 - 2w_{13}w_{23})t^2 \\ &\quad + 2(w_{03} + w_{01}w_{02}w_{03} - w_{01}w_{02}w_{12} - w_{01}w_{13} \\ &\qquad - w_{02}w_{23} + w_{03}w_{13}w_{23} - w_{12}w_{13}w_{23})t^3 \\ &\quad + (-w_{03}^2 + w_{12}^2 + 2w_{01}w_{03}w_{13} - 2w_{01}w_{12}w_{13} + 2w_{02}w_{03}w_{23} - 2w_{02}w_{12}w_{23})t^4, \end{aligned}$$

which we may use in (4.1) to conclude that the weights of the parts of the cycles in G_2 which lie in M are w_{03}, w_{12}^2, $w_{01}w_{02}$, $w_{13}w_{23}$, $w_{01}w_{13}$ and $w_{02}w_{23}$.

The first two of these are weights of cycles entirely in M, while the last four are weights of acyclic paths in M terminating at vertices of G_1. Condition (*iii*) in the Unitarity Theorems forces

$$\begin{aligned} 0 &= w_{01}w_{02} \\ 0 &= w_{13}w_{23} \\ 0 &= w_{01}w_{13} \\ 0 &= w_{02}w_{23}. \end{aligned} \tag{4.5}$$

Recall that $w_{\alpha\beta} := \langle\!\langle\alpha|\beta\rangle\!\rangle$, so that $w_{\alpha\beta} = 0$ means that $|\alpha\rangle\!\rangle$ and $|\beta\rangle\!\rangle$ are orthogonal. Thus the only solutions to (4.5) satisfy exactly one of the following sets of relations:

$$|00\rangle\!\rangle \perp |01\rangle\!\rangle \ \wedge \ |10\rangle\!\rangle \perp |11\rangle\!\rangle \tag{4.6a}$$

$$|00\rangle\!\rangle \perp |10\rangle\!\rangle \ \wedge \ |01\rangle\!\rangle \perp |11\rangle\!\rangle, \tag{4.6b}$$

where $\wedge$ is the boolean relation 'and'. These two sets of relations transform into one another under the action of P; hence we need only consider one, say (4.6*a*).

To obtain a periodic QCA, condition (*ii*) of Theorem 3.9 must also be satisfied, *i.e.*, for the cycles in M:

$$0 = w_{03} \tag{4.7a}$$

$$0 = w_{12}^2. \tag{4.7b}$$

Since the amplitude vectors for a binary CA lie in $\mathbb{C}^2$ and by (4.3) are nonzero, no more than two can be mutually orthogonal. This means that the constraints (4.7) restrict (4.6*a*) to the single frame:

$$|00\rangle\!\rangle \parallel |10\rangle\!\rangle \ \perp \ |01\rangle\!\rangle \parallel |11\rangle\!\rangle, \tag{4.8}$$

where by *frame* we mean a pair S_0, S_1 of sets of vectors in $\mathbb{C}^2$ such that each vector in S_0 is orthogonal to each vector in S_1. We will denote the family of local rules satisfying the relations (4.8) subject to the normalization constraints (4.3) by $f_{2,1}$: the subscript 2 is k; the 1 indicates that local configurations $i_{-k/2}\ldots i_{-1}i_1\ldots i_{k/2}$ with the same state i_1 have parallel amplitude vectors. An explicit parameterization of this local rule gives the rule table for $f_{2,1}(i|\lambda)$:

$f_{2,1}$	0	1
00	$e^{i\alpha}\cos\theta$	$e^{i\beta}i\sin\theta$
01	$e^{i\phi_1}\rho e^{-i\beta}i\sin\theta$	$e^{i\phi_1}\rho e^{-i\alpha}\cos\theta$
10	$e^{i\phi_2}\rho^{-1}e^{i\alpha}\cos\theta$	$e^{i\phi_2}\rho^{-1}e^{i\beta}i\sin\theta$
11	$e^{-i\beta}i\sin\theta$	$e^{-i\alpha}\cos\theta$

(4.9)

where λ labels the rows and i the columns. The four entries in rows 00 and 11 form an arbitrary $SU(2)$ matrix: $\alpha,\beta,\theta\in[0,2\pi)$; the remaining degree of freedom is an overall phase which has been divided out as it has no effect on probabilities. $|10\rangle\!\rangle$ is parallel to $|00\rangle\!\rangle$, differing by an arbitrary factor $\rho^{-1}e^{i\phi_2}\in\mathbb{C}$. $|01\rangle\!\rangle$ is parallel to $|11\rangle\!\rangle$ with length ρ and phase angle $\phi_1\in[0,2\pi)$. The only other possible periodic local rule, satisfying (4.6b), is the the parity transform: $f_{2,-1}=Pf_{2,1}$, obtained by interchanging the middle two rows in (4.9). The state transposition τ leads to no new rules: $\tau_{\rm in}$ is implemented by $\alpha\to\pi/2-\beta$, $\beta\to\pi/2-\alpha$, $\theta\to\pi/2-\theta$, $\phi_1\leftrightarrow\phi_2$ and $\rho\to\rho^{-1}$, while $\tau_{\rm out}$ is implemented just by $\alpha\to\pi/2+\beta$, $\beta\to\pi/2+\alpha$ and $\theta\to\pi/2-\theta$.

To obtain an infinite QCA, by Corollary 3.5 and Theorem 3.6, a local rule f must have a nonempty deterministic sector consisting of local configurations corresponding to the edges in a collection of cycles in G_1. The simplest possibility is that 0 is a quiescent state, so that $|00\rangle\!\rangle=(1,0)$. Conditions ($ii$) and ($iv$) of Theorem 3.10 impose no additional constraints beyond (4.3) and (4.5) if 00 is the only local configuration in D_f; using (4.6a) again we find the local rule $f_{2,1;00}$ (where the subscript 00 is the deterministic sector), which may be parameterized as:

$f_{2,1;00}$	0	1
00	1	0
01	0	$e^{i\phi_1}\rho$
10	$\rho^{-1}e^{i\alpha}\cos\theta$	$\rho^{-1}e^{i\beta}i\sin\theta$
11	$e^{i\phi_3}e^{-i\beta}i\sin\theta$	$e^{i\phi_3}e^{-i\alpha}\cos\theta$

(4.10)

since $|01\rangle\!\rangle$ is orthogonal to $|00\rangle\!\rangle$, with arbitrary nonzero component $\rho e^{i\phi_1}\in\mathbb{C}$, while the entries in rows 10 and 11 would form an arbitrary $U(2)$ matrix $\Phi^{(1)}$ but for the length ρ^{-1} of $|10\rangle\!\rangle$: $\alpha,\beta,\phi_1,\phi_3,\theta\in[0,2\pi)$ and the overall phase has been set by the choice $|00\rangle\!\rangle=(1,0)$. Finally, surjectivity constraint (i) of Theorem 3.18 requires in addition that

$f(0|10) \neq 0$, *i.e.*, $\cos\theta \neq 0$; surjectivity constraint (*ii*) is already satisfied because of the orthogonality relations. Again, the parity transform $f_{2,-1;00} = Pf_{2,1;00}$ is also a solution.

Condition (*ii*) of Theorem 3.10 will impose additional constraints only if the vertex labelled 1 in Figure 1 is also in D_1. This occurs if $\{00, 11\} \subset D_f$ or $\{00, 01, 10\} \subset D_f$. In either case $w_1 = 1 = w_2$, since $\ldots 01 \ldots$ and $\ldots 10 \ldots$ are admissible configurations in the former and $\ldots 0101 \ldots$ is an admissible configuration in the latter. Furthermore, in the first case $D_2 \cap M$ contains the cycles with weights w_{03} and in the second case the one with weight w_{01}^2, so condition (*iv*) of Theorem 3.10 imposes constraint (4.7*a*) or (4.7*b*), respectively, either of which restricts (4.6*a*) to (4.8). This leaves only the completely deterministic limit $\theta = 0 = \alpha = \phi_1 = \phi_2$, $\rho = 1$ of the periodic rule (4.9), which we will denote by $f_{2,1;D}$ (the subscript D indicates that the rule is completely deterministic), together with its parity transform. Injectivity implies surjectivity in this case [32,33], so Theorem 3.18 imposes no additional constraints.

Starting with 0 being an 'anti-quiescent' state, *i.e.*, $|00\rangle\!\rangle = (0, 1)$, forces $11 \in D_f$ immediately and leads by exactly the same argument to the limit $\theta = \pi/2 = \beta, \phi_1 = \phi_2 = 0, \rho = 1$ of (4.9), which is again completely deterministic and is immediately identifiable as both $\tau_{\text{in}} f_{2,1;D}$ and $\tau_{\text{out}} f_{2,1;D}$.

This discussion could be repeated starting with 1 as a 'quiescent' state and would lead to the $\tau_{\text{in}}\tau_{\text{out}}$ transformation of the infinite QCA rules found in the previous three paragraphs.

The last possibility for an infinite QCA is for D_f to contain only the edges 01 and 10 which form a cycle in G_1. By condition (*iv*) of Theorem 3.10, (4.7*b*) must be satisfied, *i.e.*, $\langle\!\langle 01|10\rangle\!\rangle = 0$, so again (4.6*a*) is restricted to (4.8) and we are left with exactly the same completely deterministic limits already discussed.

Note that these four deterministic CAs: $f_{2,1;D}$, $Pf_{2,1;D}$, $\tau_{\text{in}} f_{2,1;D}$ and $P\tau_{\text{in}} f_{2,1;D}$, are trivial in the sense that the local rule depends on only one of the cell states in the local configuration, *i.e.*, $f_{2,1;D}(i|i_1 i_2) = \delta_{i i_2}$. That the only deterministic binary CAs with neighborhoods of size 2 or 3 are trivial in this sense is well known [35] (this is also the sense in which the only linear QCAs which are allowed by the No-Go Theorem are trivial for *any* size neighborhood [8]); we have just shown that if D_f contains more than just 00 (or 11) then infinite $k = 2$ QCAs are trivial in the same way. It is most interesting that when $D_f = \{00\}$ (or $\{11\}$) the local rule is not completely deterministic and, furthermore, partitions the amplitude vectors into two independent frames rather than the single frame of the periodic local rules.

4.2. $k = 3$

The next simplest binary CAs have local neighborhoods of size 3. Figure 3 shows G_1 (in this subsection the arguments $Q = \{0, 1\}$ and $k = 3$ are suppressed). The cycles may be determined as in the previous subsection; then condition (*i*) of the Unitarity Theorems

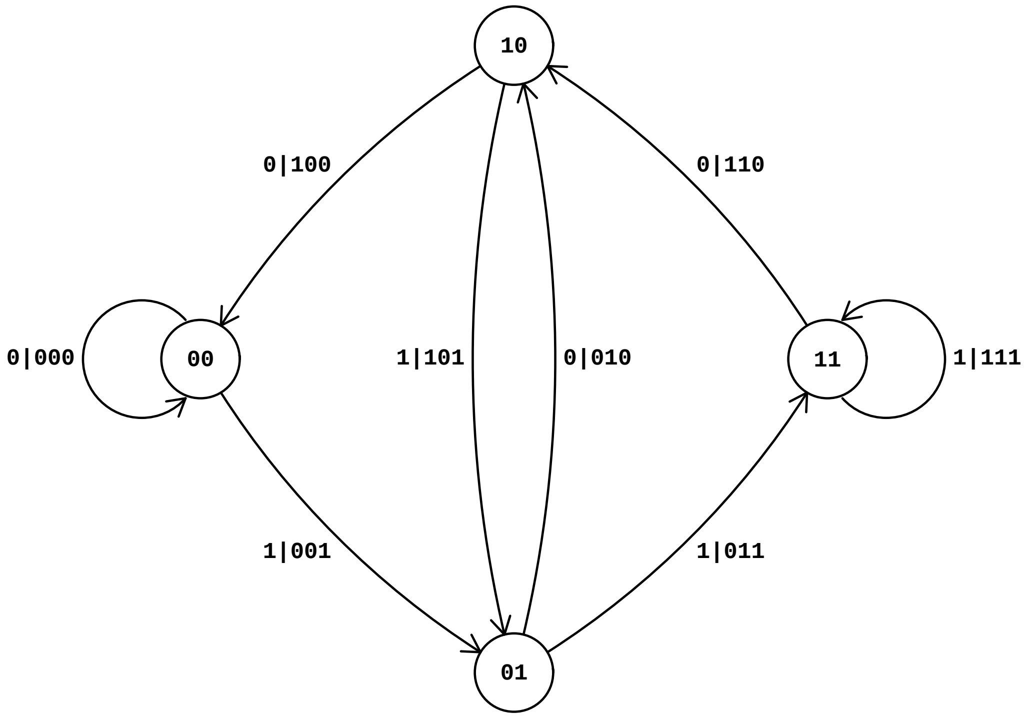

Figure 3. G_1 for binary CAs with local neighborhoods of size 3.

imposes the constraints:

$$\begin{array}{lll} 1 = w_0 & 1 = w_2 w_5 & 1 = w_3 w_6 w_5 \\ 1 = w_7 & 1 = w_1 w_2 w_4 & 1 = w_1 w_3 w_6 w_4. \end{array} \tag{4.11}$$

Note that only the first five of these constraints are independent: reading the columns left to right, the last equation is implied by the three preceding.

G_2 is quite complicated to draw, but by computing successive powers of A_2 (now a 16×16 matrix, so computing the determinant in $Z_2(t)$ is tedious, even by computer), we find the weights of the parts of the acyclic paths of length $n \leq 4$ in M terminating at vertices of G_1; they are listed in Appendix A. Condition (*iii*) in the Unitarity Theorems requires that each of these weights vanish. The only solutions to these constraints satisfy one of the following sets of relations:

$$|000\rangle\!\rangle \perp |001\rangle\!\rangle \ \wedge\ |010\rangle\!\rangle \perp |011\rangle\!\rangle \ \wedge\ |100\rangle\!\rangle \perp |101\rangle\!\rangle \ \wedge\ |110\rangle\!\rangle \perp |111\rangle\!\rangle \tag{4.12a}$$

$$|000\rangle\!\rangle \perp |100\rangle\!\rangle \ \wedge\ |010\rangle\!\rangle \perp |110\rangle\!\rangle \ \wedge\ |001\rangle\!\rangle \perp |101\rangle\!\rangle \ \wedge\ |011\rangle\!\rangle \perp |111\rangle\!\rangle \tag{4.12b}$$

$$|000\rangle\!\rangle \parallel |100\rangle\!\rangle \perp |010\rangle\!\rangle \parallel |110\rangle\!\rangle \ \wedge\ |001\rangle\!\rangle \parallel |101\rangle\!\rangle \perp |011\rangle\!\rangle \parallel |111\rangle\!\rangle \tag{4.12c}$$

$$|000\rangle\!\rangle \parallel |001\rangle\!\rangle \perp |010\rangle\!\rangle \parallel |011\rangle\!\rangle \ \wedge\ |100\rangle\!\rangle \parallel |101\rangle\!\rangle \perp |110\rangle\!\rangle \parallel |111\rangle\!\rangle. \tag{4.12d}$$

That any of these sets of relations implies that the weights of *all* acyclic paths of *any* length in M terminating at vertices of G_1 vanish is a consequence of Theorem 5.1 (which

is stated and proved in the next section). Just as in the $k = 2$ case, the second and fourth sets of relations are merely the parity transforms of the first and third, respectively, so we need only consider the possibilities (4.12a) and (4.12c).

To obtain a periodic QCA, condition (ii) of Theorem 3.9 must also be satisfied, *i.e.*, we must consider the cycles in M. There are four cycles of length $n \le 2$, with weights: w_{07}, w_{25}^2, $w_{02}w_{05}$ and $w_{27}w_{57}$. Of the eight cycles of length $n = 3$, four are contained entirely in M, with weights: $w_{03}w_{05}w_{06}$, $w_{12}w_{14}w_{24}$, $w_{17}w_{27}w_{47}$ and $w_{35}w_{36}w_{56}$; the other four are acyclic paths terminating at vertices in G_1 and so are already included in the list in Appendix A. Imposing the constraint that each of these weights vanish implies that the relations (4.12a) are restricted to a single frame:

$$|000\rangle\!\rangle \parallel |010\rangle\!\rangle \parallel |100\rangle\!\rangle \parallel |110\rangle\!\rangle \perp |001\rangle\!\rangle \parallel |011\rangle\!\rangle \parallel |101\rangle\!\rangle \parallel |111\rangle\!\rangle, \qquad (4.13a)$$

while the relations (4.12c) are restricted to the frame:

$$|000\rangle\!\rangle \parallel |001\rangle\!\rangle \parallel |100\rangle\!\rangle \parallel |101\rangle\!\rangle \perp |010\rangle\!\rangle \parallel |011\rangle\!\rangle \parallel |110\rangle\!\rangle \parallel |111\rangle\!\rangle. \qquad (4.13c)$$

Note that (4.13c) is invariant under parity reversal (and hence is also the consequence of (4.12d)), while (4.13a) is not (and hence (4.12b) leads to its parity transform). These three frames are the only possibilities for local rules. To show that the longer cycles in G_2 rule out none of them, consider one and write the transition matrix A_2, as in (4.4), with 0s for the weights which vanish in the given frame. The resulting matrix is sufficiently sparse that $Z_2(t) = \det(I - tA_2)$ can be computed easily. In each of these frames we find that $Z_2(t) = 1 - t^2 - 2t^3 - t^4$. Since we may compute $\mathrm{Tr}A_2(t)$ from $Z_2(t)$ by (4.1), this means that there are no further orthogonality constraints on the weights.

Thus (4.13a) subject to the normalization constraints (4.11) gives a local rule $f_{3,1}$ (for k odd we label the local configuration $i_{-(k-1)/2} \ldots i_0 \ldots i_{(k-1)/2}$; the subscript 1 again indicates that the frame in (4.13a) partitions the amplitude vectors according to i_1 in the local configuration). A more concise description of this local rule than an explicit parameterization like (4.9) is that the amplitude vectors for $f_{3,1}$ satisfy:

$$\begin{aligned}
&|000\rangle\!\rangle \text{ and } |111\rangle\!\rangle \text{ form an orthonormal basis of } \mathbb{C}^2 \\
&|010\rangle\!\rangle = z_2|000\rangle\!\rangle,\ |100\rangle\!\rangle = z_4|000\rangle\!\rangle,\ |110\rangle\!\rangle = z_6|000\rangle\!\rangle \\
&|001\rangle\!\rangle = z_1|111\rangle\!\rangle,\ |011\rangle\!\rangle = z_3|111\rangle\!\rangle,\ |101\rangle\!\rangle = z_5|111\rangle\!\rangle \\
&z_i \in \mathbb{C}, i \in \{1,\ldots,6\};\ |z_2z_5| = 1,\ |z_1z_2z_4| = 1,\ |z_3z_5z_7| = 1.
\end{aligned} \qquad (4.14a)$$

The amplitude vectors satisfying the constraints (4.13c) subject to the normalization constraints (4.11) may be described similarly, changing the middle two lines of (4.14a) to:

$$\begin{aligned}
&|001\rangle\!\rangle = z_1|000\rangle\!\rangle,\ |100\rangle\!\rangle = z_4|000\rangle\!\rangle,\ |101\rangle\!\rangle = z_5|000\rangle\!\rangle \\
&|010\rangle\!\rangle = z_2|111\rangle\!\rangle,\ |011\rangle\!\rangle = z_3|111\rangle\!\rangle,\ |110\rangle\!\rangle = z_6|111\rangle\!\rangle.
\end{aligned} \qquad (4.14c)$$

We denote this rule by $f_{3,0}$. Finally, the parity transform $f_{3,-1} = Pf_{3,1}$ gives the solution corresponding to (4.12b). Each of these rules may be parameterized by 12 real parameters

and an overall phase: 6 for the first pair of orthogonal vectors, 2 for each additional vector in the frame, and -1 for each independent normalization constraint. These are all the rule families for the periodic case; just as when $k = 2$ the state transposition τ leads to no additional rules.

For an infinite QCA, the possible deterministic sectors are determined by the cycles in G_1. Viewing Figure 3 or recalling (4.11), we see that the sets of local configurations appearing in cycles are: $\{000\}$, $\{111\}$, $\{010, 101\}$, $\{001, 010, 001\}$, $\{011, 101, 110\}$ and $\{001, 011, 100, 110\}$; any union of one or more of these sets is a possibility for D_f.

The simplest possibility is $D_f = \{000\}$, *i.e.*, 0 is uniquely quiescent. In this case $|000\rangle\!\rangle = (1, 0)$ and conditions (*ii*) and (*iv*) of Theorem 3.10 impose no additional constraints beyond (4.11) and (4.12). (4.12a) defines the rule family denoted $f_{3,1;000}$ with amplitude vectors partitioned into four frames:

$$\begin{aligned}
&|000\rangle\!\rangle = (1, 0);\ |001\rangle\!\rangle = (0, z_1)\\
&|\alpha 0\rangle\!\rangle \text{ and } |\alpha 1\rangle\!\rangle \text{ are orthogonal for } \alpha \in \{01, 10, 11\}\\
&\text{the norms of the amplitude vectors satisfy (4.11),}
\end{aligned} \tag{4.15a}$$

a 16 real parameter family of local rules. Surjectivity constraint (*i*) of Theorem 3.18 rules out only the codimension 1 submanifolds defined by $f(0|010) = 0$, $f(0|100) = 0$ and $f(0|110) = 0$, while surjectivity constraint (*ii*) is again satisfied as a consequence of the orthogonality relations. Similarly, (4.12c) would define a rule family with amplitude vectors satisfying:

$$\begin{aligned}
&|000\rangle\!\rangle = (1, 0);\ |001\rangle\!\rangle = (z_1, 0);\ |010\rangle\!\rangle = (0, z_2);\ |011\rangle\!\rangle = (0, z_3)\\
&|10i\rangle\!\rangle \text{ and } |11j\rangle\!\rangle \text{ are orthogonal for } i, j \in \{0, 1\}\\
&\text{the norms of the amplitude vectors satisfy (4.11),}
\end{aligned} \tag{4.15c}$$

except that $|010\rangle\!\rangle = (0, z_2)$ conflicts with the surjectivity constraint that $f(0|010) = 0$, ruling out this possibility. Thus $f_{3,1;000}$ and its distinct parity transform are the only allowed rule families when $D_f = \{000\}$. Both of these infinite QCAs with 0 uniquely quiescent have distinct state transposition transforms under $\tau_{\text{in}}\tau_{\text{out}}$ with 1 as a 'quiescent' state.

The next simplest possibility is that $D_f = \{000, 111\}$. Then by condition (*ii*) of Theorem 3.10, the two acylic paths in G_1 terminating at 000 and 111 must each have weight 1:

$$\begin{aligned}
1 &= w_1 w_3\\
1 &= w_4 w_6.
\end{aligned} \tag{4.16}$$

With (4.11), the second of these constraints is implied by the first. By condition (*iv*) of Theorem 3.10, the cycles in $D_2 \cap M$ must have vanishing weights. Hence $0 = w_{07}$. This constraint restricts (4.12a) to the three frame set of relations:

$$|000\rangle\!\rangle \parallel |110\rangle\!\rangle \perp |001\rangle\!\rangle \parallel |111\rangle\!\rangle \ \wedge\ |010\rangle\!\rangle \perp |011\rangle\!\rangle \ \wedge\ |100\rangle\!\rangle \perp |101\rangle\!\rangle \tag{4.17a}$$

and restricts (4.12c) to (4.13c). We define the rule $f_{3,1;000,111}$ by the set of amplitude vectors satisfying (4.17a) subject to the normalization constraints (4.11) and (4.16) and with $D_f = \{000, 111\}$, described by:

$$
\begin{aligned}
&|000\rangle\!\rangle = (1,0);\ |110\rangle\!\rangle = (z_3,0),\ |001\rangle\!\rangle = (0,z_1);\ |111\rangle\!\rangle = (0,1)\\
&|\alpha 0\rangle\!\rangle \text{ and } |\alpha 1\rangle\!\rangle \text{ are orthogonal for } \alpha \in \{01,10\}\\
&\text{the norms of the amplitude vectors satisfy (4.11) and (4.16),}
\end{aligned}
$$

a 12 real parameter family of local rules. Surjectivity condition (ii) of Theorem 3.18 restricts these parameter values by removing the codimension 1 submanifolds defined by $f(0|010) = 0$, $f(0|100) = 0$, $f(1|011) = 0$ and $f(1|101) = 0$. Surjectivity condition (ii) is ensured by the orthogonality of $|\alpha 0\rangle\!\rangle$ and $|\alpha 1\rangle\!\rangle$ for all $\alpha \in Q^2$. $f_{3,1;000,111}$ has a distinct parity transform but is invariant under $\tau_{\rm in}\tau_{\rm out}$. Applying either of the state transposition transforms alone produces a distinct rule family in which 0 is 'anti-quiescent', as is 1.

The rule which would be defined by (4.14c) with $|000\rangle\!\rangle = (1,0)$ and $|111\rangle\!\rangle = (0,1)$ is ruled out by surjectivity condition (i) of Theorem 3.18: $|010\rangle\!\rangle = (0,z_2)$ contradicts $f(0|010) \neq 0$, for example. Similarly, $|000\rangle\!\rangle = (0,1)$ and $|111\rangle\!\rangle = (1,0)$ fails to be surjective: in this case $|010\rangle\!\rangle = (z_2,0)$ contradicts $f(1|010) \neq 0$.

We may continue to increase the size of D_f and find further infinite QCA rules; the procedure is clear. When the deterministic sector gets only a little larger, there will be only completely deterministic rules, just as in the $k = 2$ case of the previous subsection.

5. Discussion

The results of the previous section demonstrate that the Unitarity Theorems provide an effective procedure for finding one dimensional binary QCAs, both periodic and infinite. Although it is increasingly difficult to find the most general unitary solutions for large local neighborhood size k—the procedure is not very efficient—the results for $k = 2$ and $k = 3$ suggest a pattern for some *particular* solutions. Specifically, the sets of relations (4.6) and (4.12) generalize to larger values of k. If we generalize the notion of 'frame' to q-*frame*: a collection $S_0,\ldots,S_{q-1}$ of sets of vectors in $\mathbb{C}^q$ such that each vector in S_i is orthogonal to each vector in S_j for $i \neq j$, we can state the following:

THEOREM 5.1. *Let $0 < j < k \in \mathbb{Z}$. For each $\gamma \in Q^j$ define a q-frame*

$$S^{(\gamma)} = \{S_0^{(\gamma)},\ldots,S_{q-1}^{(\gamma)}\}$$

by

$$S_i^{(\gamma)} = \{|i_i \ldots i_k\rangle\!\rangle \mid i_1 \ldots i_j = \gamma, i_{j+1} = i \in Q\}.$$

Then condition (iii) of the Unitarity Theorems—the weight of any acyclic path in $M(Q,k)$ terminating at vertices in $G_1(Q,k)$ vanishes—holds when the amplitude vectors are partitioned into the q^j frames $\{S^{(\gamma)}\}$, or into their parity transforms.

Proof. Consider any acyclic path in $M(Q,k)$ starting from a vertex $(\alpha,\alpha) \in G_1(Q,k) \subset G_2(Q,k)$, where $\alpha \in Q^{k-1}$. The $(k-j)^{\text{th}}$ edge in the path is necessarily labelled

$$(i_1 \ldots i_j i''_{j+1} \ldots i''_k, i_1 \ldots i_j i'_{j+1} \ldots i'_k),$$

where $i_1 \ldots i_j$ are the rightmost j states in α and $i''_{j+1} \neq i'_{j+1}$ since the first edge of the path would not lie in $M(Q,k)$ otherwise. Let $\gamma = i_1 \ldots i_j$; then $|i_1 \ldots i_j i''_{j+1} \ldots i''_k\rangle\!\rangle \in S^{(\gamma)}_{i''_{j+1}}$ and $|i_1 \ldots i_j i'_{j+1} \ldots i'_k\rangle\!\rangle \in S^{(\gamma)}_{i'_{j+1}}$. Since all the amplitude vectors in $S^{(\gamma)}_{i''}$ are orthogonal to those in $S^{(\gamma)}_{i'}$ for $i'' \neq i'$,

$$\langle\!\langle i_1 \ldots i_j i''_{j+1} \ldots i''_k | i_1 \ldots i_j i'_{j+1} \ldots i'_k\rangle\!\rangle = 0$$

and the weight of the path vanishes. To show that the parity transformed set of frames $P\{S^{(\gamma)}\}$ also enforces condition (iii) of the Unitarity Theorems, make the analogous argument using the terminal vertex of the acyclic path rather than its initial vertex. ∎

The special case $q = 2$ and $k = 3$ of Theorem 5.1 shows that each of the sets of relations (4.12) which were found by considering only acyclic paths of length $n \leq 4$ implies that the weights of all acyclic paths of any length in $M(\{0,1\},3)$ terminating at vertices of $G_1(\{0,1\},3)$ vanish; (4.12a) and (4.12b) are parity dual sets of frames for $j = 2$, while (4.12c) and (4.12d) are the parity dual sets of frames for $j = 1$.

That the converse of Theorem 5.1 is false is demonstrated by the existence of the nontrivial $k = 4$ *reversible* deterministic CA found by Patt [36], with local rule:

$$f(i|i_1 i_2 i_3 i_4) = \begin{cases} 1 - \delta_{ii_2} & \text{if } i_1 = i_4 = 0,\ i_3 = 1; \\ \delta_{ii_2} & \text{otherwise.} \end{cases}$$

Reversible CAs are *a fortiori* unitary and this local rule partitions the $k = 4$ amplitude vectors inconsistently with each of the sets of frames described in Theorem 5.1.

Consideration of this example leads to the observation that any reversible deterministic CA can be ‘quantized’: The local rule of such a CA partitions the amplitude vectors $|i_1 \ldots i_k\rangle\!\rangle$ into a single q-frame according to the unique $i \in Q$ for which $f(i|i_1 \ldots i_k)$ is nonzero. Any rigid rotation of $\mathbb{C}^q$ preserves this q-frame, and hence unitarity, but gives, generically, nonzero transition amplitudes for all the $f(i|i_1 \ldots i_k)$. The resulting global evolution is unitarily inequivalent to the original reversible deterministic evolution.

Although the local rules for the periodic QCAs found in Section 4 also partition the amplitude vectors into a single frame (see (4.8) and (4.13)), they have additional degrees of freedom associated with the lengths of the amplitude vectors: 1 when $k = 2$ and 3 when $k = 3$; this should be contrasted with deterministic local rules for which all the amplitude vectors have length 1. Despite being asymptotically deterministic, the infinite QCAs with local rules found in Section 4 are even further from the deterministic situation;

their amplitude vectors lie in more than a single frame: as many as 2^{k-1} for some of the QCAs with 0 uniquely quiescent (see (4.10) and (4.15a)).

The multidimensionality of the local rule spaces for even the small neighborhood QCAs we have considered suggests that binary QCAs may have a wide range of quantum behaviors/computational power. Whether any are computationally universal remains to be discovered. There is a long standing conjecture that computational power will be maximal at critical points of a physical theory [37]. Since the rule spaces here are smoothly parameterized this is a more natural arena in which to investigate this conjecture than is the deterministic case.

Consideration of QCAs as physical models, possibly with critical points, raises the question of the continuum limits of these models. The simplest nontrivial* one dimensional linear binary QCAs have the $1+1$ dimensional Dirac equation as their continuum limit [9]. From the perspective of fundamental physics, it would be most interesting to determine the continuum limits of the simple nonlinear models we have found here and to extend them to higher dimensions. That the reversible deterministic billiard ball model is computational universal [38] suggests that higher dimensional QCAs might also be easier to prove computationally powerful. It should be noted, however, that there can be no analogue of the Unitarity Theorems in higher dimensions since reversibility of deterministic CAs is undecidable in two dimensions [39]; the best we can expect is, as in Theorem 5.1, to find particular sets of local rules which ensure unitarity.

Despite the existence of computation universal deterministic CAs, probably their most important applications are simulations of physical systems [40]. Similarly, it seems likely that QCAs will prove optimally suited not to universal computation but for the simulation of specific quantum mechanical systems and the solution of particular classes of problems.

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* Recall that the No-go Theorem requires that the QCA not be homogeneous if it is to be nontrivial.

Appendix A

The weights of the acyclic paths of length $n \leq 4$ in $M(\{0,1\},3)$ terminating at vertices of $G_1(\{0,1\},3)$ are:

$n = 3$:

$$
\begin{array}{llll}
w_{01}w_{02}w_{04} & w_{01}w_{02}w_{15} & w_{01}w_{13}w_{26} & w_{01}w_{13}w_{37} \\
w_{02}w_{04}w_{45} & w_{02}w_{15}w_{45} & w_{13}w_{26}w_{45} & w_{13}w_{37}w_{45} \\
w_{04}w_{23}w_{46} & w_{15}w_{23}w_{46} & w_{23}w_{26}w_{57} & w_{23}w_{37}w_{57} \\
w_{04}w_{46}w_{67} & w_{15}w_{46}w_{67} & w_{26}w_{57}w_{67} & w_{37}w_{57}w_{67}
\end{array}
$$

$n = 4$:

$$
\begin{array}{llll}
w_{01}w_{03}w_{04}w_{06} & w_{01}w_{03}w_{06}w_{15} & w_{01}w_{04}w_{12}w_{24} & w_{01}w_{12}w_{15}w_{24} \\
w_{01}w_{03}w_{17}w_{26} & w_{01}w_{12}w_{26}w_{35} & w_{01}w_{03}w_{17}w_{37} & w_{01}w_{12}w_{35}w_{37} \\
w_{03}w_{04}w_{06}w_{45} & w_{03}w_{06}w_{15}w_{45} & w_{04}w_{12}w_{24}w_{45} & w_{12}w_{15}w_{24}w_{45} \\
w_{03}w_{17}w_{26}w_{45} & w_{12}w_{26}w_{35}w_{45} & w_{03}w_{17}w_{37}w_{45} & w_{12}w_{35}w_{37}w_{45} \\
w_{04}w_{06}w_{23}w_{47} & w_{06}w_{15}w_{23}w_{47} & w_{17}w_{23}w_{26}w_{47} & w_{17}w_{23}w_{37}w_{47} \\
w_{04}w_{23}w_{24}w_{56} & w_{15}w_{23}w_{24}w_{56} & w_{23}w_{26}w_{35}w_{56} & w_{23}w_{35}w_{37}w_{56} \\
w_{04}w_{06}w_{47}w_{67} & w_{06}w_{15}w_{47}w_{67} & w_{17}w_{26}w_{47}w_{67} & w_{17}w_{37}w_{47}w_{67} \\
w_{04}w_{24}w_{56}w_{67} & w_{15}w_{24}w_{56}w_{67} & w_{26}w_{35}w_{56}w_{67} & w_{35}w_{37}w_{56}w_{67}.
\end{array}
$$

These are determined by $(A_2^3)_{ij}$ and $(A_2^4)_{ij}$, respectively, where $i, j \in \{(00,00),(01,01),(10,10),(11,11)\}$, since this is the set of labels for the vertices in G_2 which lie in the subgraph isomorphic to G_1.

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